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Re: Grant No. N00014-89-J-2038

Dear Sirs,

Please find attached my "final report" for Grant No. N00014-89-J-2038.
Copies of the final report have been sent off to the Scientific Officer at Naval
Research Laboratory and the Director at NRL.

Yours sincerely,

L. R. Ram Mohan

L. R. Ram-Mohan
Professor of Physics
& Electrical Engineering

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cc: ONR Resident Representative
MIT, Cambridge, MA 02139

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Final Report to the Naval Research Laboratory
on Research Grant: N00014-89-J-2038
Title: "Band Structure and Optical Properties of Semiconductor
Superlattices"

L. R. Ram-Mohan
Department of Physics
Worcester Polytechnic Institute

The NRL through SDI-ISTO has supported this project at WPI during 1989-1991, providing support for 1 graduate student at WPI.

This period has been very productive in terms of research results, as evidenced by 13 publications on magneto-optics and magneto-transport in collaboration with the NRL research group.

I. The Transfer Matrix Algorithm:

The theoretical development of the transfer matrix method (TMM) by me has provided a compact and efficient algorithm for the band structure of superlattices.

- It has been the mainstay in the interpretation of experimental data on magneto-optics and magneto-transport in zero-gap superlattices of HgTe/CdTe at three institutions: NRL, Notre Dame, and MIT. A complete picture has emerged which is able to explain the observed magneto-optical spectra by including contributions throughout the entire superlattice Brillouin zone.
- The analysis of piezomodulation studies at Purdue was also performed using this method. Parabolic well heterostructures were studied using piezomodulation which revealed a rich spectrum of transitions all the way from the spin-orbit split-off band quantum well levels to the conduction band levels. The theory work was done at WPI.
- Theoretical investigations at WPI of the optical nonlinearity $\chi^{(3)}$ in superlattices of *GaAs/AlGaAs* have been based on the TMM. We have investigated in a systematic manner the issue of determining the optimal widths for the wells and barriers in order to increase the optical nonlinearity.

- Work was done at NRL on investigating effects of lateral confinement in very narrow-gap superlattices, using the TMM algorithm to induce the lateral confinement through the use of a magnetic field. This has led to predictions of an energy level spectrum in such materials which displays unusual features in energy level spacing and level-filling effects which suggest that resistance quantization is not an integral multiple of the fundamental factor of $2e/h$.
- More recent work at the NRL has predicted a magnetic field induced transition from semiconducting to semimetallic behaviour at zero temperature in narrow-gap semiconductors. Again, this work was made feasible through the TMM.
- As promised in the proposal, the ability to study superlattice structures with arbitrary growth direction was implemented in the TMM algorithm. Calculations on type I and II superlattices with arbitrary growth direction, with built-in strain, and in the presence of external magnetic field, can now proceed ahead.

At present the TMM is capable of including effects of (i) a magnetic field applied perpendicular to the layers, (ii) strain in the layers for any III-V or II-VI layered quantum heterostructures. The following items need to be studied.

- *Modulation doping and a selfconsistent calculation of band bending in superlattices and quantum wells*
So far I have studied the issues and problems in a one-band model. The experience suggests that I should use the finite element method for this problem (see below). This is being investigated at present by me.
- *Quantum Wells*
The 8-band TMM has been set up for superlattices only. It is important to implement the programs for quantum wells as well. *Over the past 3 months I have been able to (i) clarify why the TMM algorithm has some instabilities which create vexing problems for calculations with it (this is due to the presence of spurious states, which can be identified and eliminated); (ii) develop the theoretical model for the calculation of energy levels in quantum wells.* These two developments in the theory of the TMM suggest that I should review the programs and up-date them in the light of the accumulated experience over the past 3 years with the TMM.
- Work is in progress to extend its applicability to modulation doping and to electric field effects.

The student supported by NRL has also been working on the issues of developing tight-binding models and algorithms for the investigation of (i) band structures of bulk III-V and II-VI semiconductors with special emphasis on evaluation of deformation potential constants at the band-edges and for intervalley scattering; (ii) the band structure of superlattices and quantum wells in very narrow layers (short-period superlattices, δ -doping effects, etc); (iii) superlattice band structures for materials with energy minima away from the Brillouin zone center, such as PbTe-PbSnTe superlattices, etc.

The list of publications is attached.

Statement A per telecon John Boores
NRL/Code 3220.TB Washington, DC 20375-5000

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Dist	Avail. to Major Special
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PUBLICATIONS DURING 1989-1991

The Transfer matrix method and its applications

1. "Double Hole Cyclotron Resonance in Zero-Gap $HgTe$ - $CdTe$ Superlattices"; J. R. Meyer, R. J. Wagner, F. J. Bartoli, C. A. Hoffman, and L. R. Ram-Mohan, *Phys. Rev. B* **40**, *Rapid Communications*, 1388-1391 (1989).
2. "The Effect of Conduction Band Nonparabolicity in $GaAs/Ga_{1-x}Al_xAs$ Semiconductor Quantum Wells"; K. H. Yoo, L. R. Ram-Mohan, and D. F. Nelson, *Physical Review B* **39**, 12808-12813 (1989).
3. "Far Infrared Magneto-optical Study of Holes and Electrons in Zero-gap $HgTe/Cd_{0.85}Hg_{0.15}Te$ Superlattices"; M. Dobrowolska, T. Wojtowicz, H. Luo, J. K. Furdyna, O. K. Wu, J. R. Meyer, C. A. Hoffman, F. J. Bartoli and L. R. Ram-Mohan, *Semicond. Sci. Technol.* **5**, s103-s106 (1990).
4. "Room Temperature Magnetoabsorption in $HgTe/Hg_{0.15}Cd_{0.85}Te$ Superlattices"; K. H. Yoo, R. L. Aggarwal, L. R. Ram-Mohan, and O. K. Wu, *J. Vac. Sci. Technol. A* **8**, 1194-1199 (1990).
5. "Electron Transport and Cyclotron Resonance in [211]-Oriented $HgTe$ - $CdTe$ Superlattices"; C. A. Hoffman, J. R. Meyer, R. J. Wagner, F. J. Bartoli, X. Chu, J. P. Faurie, L. R. Ram-Mohan, and H. Xie, *J. Vac. Sci. Technol. A* **8**, 1200-1205 (1990).
6. "Band edge properties of quasi-1D $HgTe/CdTe$ heterostructures"; J. R. Meyer, F. J. Bartoli, C. A. Hoffman, and L. R. Ram-Mohan, *Physical Review Letters* **64**, 1963-1966 (1990).
7. "Stimulated Emission of Longitudinal Optic Phonons in Narrow Gap $Pb_{1-x}Sn_xTe$ "; R. B. Sohn, L. R. Ram-Mohan, H. Xie, and P. A. Wolff, *Physical Review B* **42**, 3608-3619 (1990).
8. "Electron Hole Recombination in Narrow Gap $Hg_{1-x}Cd_xTe$ and Stimulated Emission of Longitudinal Optic Phonons"; H. Xie, L. R. Ram-Mohan, and P. A. Wolff, *Physical Review B* **42**, 3620-3627 (1990).
9. "Nonlinear Optical Properties of $GaAs/Ga_{1-x}Al_xAs$ Superlattices"; H. Xie, L. Friedman, and L. R. Ram-Mohan, *Physical Review B* **42**, 7124-7131 (1990).
10. "Magneto-optical properties of $HgTe$ - $CdTe$ superlattices"; J. R. Meyer, F. J. Bartoli, C. A. Hoffman, and L. R. Ram-Mohan, *Physical Review B* **42**, 9050-9062 (1990).
11. "Higher-order electron cyclotron resonance in n -type $HgTe$ - $CdTe$ superlattices"; M. Dobrowolska, T. Wojtowicz, J. K. Furdyna, J. R. Meyer, R. D. Feldman, R. F. Austin, and L. R. Ram-Mohan, *Applied Physics Letters* **57**, 1781-1783 (1990).
12. "Optical nonlinearities of $GaAs/Ga_{1-x}Al_xAs$ superlattices"; H. Xie, L. Friedman, and L. R. Ram-Mohan, *SPIE Proceedings Vol 1283*, 360-371 (1990).

13. "Magneto-optical resonances in $HgTe-CdTe$ superlattices"; J. R. Meyer, F. J. Bartoli, C. A. Hoffman, M. Dobrowolska, T. Wojtowicz, J. K. Furdyna, and L. R. Ram-Mohan, *Proc. 20th Int. Conf. on the Physics of Semiconductors*; ed. E. M. Anastassakis and J. D. Joannopoulos (World Scientific, Singapore, 1990), p1170-1173 (1991).
14. "Laterally confined $HgTe-CdTe$ quantum wells and superlattices"; J. R. Meyer, F. J. Bartoli, C. A. Hoffman and L. R. Ram-Mohan, *Proc. 5th Int. Conf. on Physics of Electro-Optic Materials, 1990*, Crete, Greece, (1991).
15. "Magneto-optical transitions between subbands with different quantum numbers in narrow gap $HgTe-CdTe$ superlattices"; H. Luo, G. L. Yang, J. K. Furdyna, and L. R. Ram-Mohan, *J. Vac. Sci. Technol. B* **9**, 1809-1812 (1991).
16. "Theory for electron and hole transport in $HgTe-CdTe$ superlattices"; J. R. Meyer, D. J. Arnold, C. A. Hoffman, F. J. Bartoli, and L. R. Ram-Mohan, *J. Vac. Sci. Technol. B* **9**, 1818-1822 (1991).
17. "Laterally confined $HgTe-CdTe$ quantum wells and superlattices"; J. R. Meyer, F. J. Bartoli, C. A. Hoffmann, and L. R. Ram-Mohan, *Superlattices and Microstructures* **7**, 387-391 (1991).
18. "Magnetic activation of bipolar plasmas in $HgTe-CdTe$ superlattices"; J. R. Meyer, C. A. Hoffman, F. J. Bartoli, T. Wojtowicz, M. Dobrowolska, J. Furdyna, X. Chu, J. P. Faurie, and L. R. Ram-Mohan, *Phys. Rev. B* **44**, *Rapid Communications*, 3455-3458 (1991).

The Finite Element Method and its Applications

1. "Removal of accidental degeneracies in quantum wires"; J. Shertzer and L. R. Ram-Mohan, *Physical Review B* **41**, 9994-9999 (1990).
2. "Electronic energy bands and optical nonlinearity of checker-board superlattices"; L. R. Ram-Mohan and J. Shertzer, *Applied Physics Letters* **57**, 282-284 (1990).
3. "Observation of above-barrier quasi-bound states in asymmetric single quantum wells by piezomodulated reflectivity"; D. Dossa, Lok C. Lew yan Voon, L. R. Ram-Mohan, C. Parks, R. G. Alonso, A. K. Ramdas, and M. R. Melloch, *Applied Physics Letters* **59**, 2706-2708 (1991).